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1  #-*- coding: utf-8 -*-
2  """
3  Created on Tue Mar  5 10:48:44 2019
4
5  @author: Nate
6  """
7
8  import numpy as np
9  import matplotlib.pyplot as plt
10 import pdb
11
12 #fig2, axes2 = plt.subplots()
13
14
15 #####
16 #####
17 #defining constants
18
19 #number of trials
20 N = 10000
21
22
23 #α=0.2 to 2 in increments of 0.2
24
25 alpha = [i*.2 for i in range(1,11)]
26 rmax_list = [(2.1/alph) for alph in alpha]
27 r0 = np.array([2,2,2])
28 r1 = np.array([3,2,2])
29 energy = []
30 std_dev = []
31
32
33
34 #sigma = [4*i for i in alpha]
35 #rmax = 1/(2*alpha)
36
37
38
39
40 #####
41 #####
42 #defining functions
43
44
45 def get_delta_r(rmax):
46     delta_r =
47         np.array([rmax*(np.random.uniform()-.5), rmax*(np.random.uniform()-.5), rmax*(np.random
48             .uniform()-.5)])
49     return(delta_r)
50
51 #evaluate ratio
52 def evaluate_ratio(r, delta_r, r2, delta_r2):
53     global count
54     A = np.exp(-2*alpha[i]*np.linalg.norm(r))*np.exp(-2*alpha[i]*np.linalg.norm(r2))
55     B =
56         np.exp(-2*alpha[i]*np.linalg.norm(r+delta_r))*np.exp(-2*alpha[i]*np.linalg.norm(r2+de
57             lta_r2))
58     ratio = B/A
59
60
61     if ratio > np.random.uniform():
62         count+=1
63         return(True)
64     else:
65         return(False)
66
67 def generate_point(r, delta_r, r2, delta_r2):

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64     if evaluate_ratio(r, delta_r, r2, delta_r2) == True:
65         return(r+delta_r, r2+delta_r2)
66     else:
67         return(r, r2)
68
69
70 #####
71 #####
72
73
74
75 for i in range(len(alpha)):
76
77     #generating points
78     r = np.array([r0])
79     r2 = np.array([r1])
80     count = 0
81     en = 0
82
83     for j in range(N):
84         #r2=np.random.exponential(.5/alpha[i])
85         #en += -alpha[i]**2 + alpha[i]/np.linalg.norm(r2) - 1/np.linalg.norm(r2)
86
87         x, y = generate_point(r[len(r)-1], get_delta_r(rmax_list[i]), r2[len(r2)-1],
88                               get_delta_r(rmax_list[i]))
89
90         r = np.append(r, [x], axis = 0)
91         r2 = np.append(r2, [y], axis = 0)
92
93         #pdb.set_trace()
94         r_mag = np.linalg.norm([r[j][0], r[j][1], r[j][2]])
95         r2_mag = np.linalg.norm([r2[j][0], r2[j][1], r2[j][2]])
96         r12 = np.sqrt((r[j][0]-r2[j][0])**2 + (r[j][1]-r2[j][1])**2 +
97                       (r[j][2]-r2[j][2])**2)+.0000001
98
99         E1 = -(1/2.0)*alpha[i]**2+ alpha[i]/r_mag-2/r_mag
100        E2 = -(1/2.0)*alpha[i]**2+ alpha[i]/r2_mag-2/r2_mag
101        en += E1 + E2 + (1.0/r12)
102
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107
108    print(rmax_list[i], 'accepted: ', count, 'rejected: ', N-count)
109    print('Acceptance Ratio: ', count/N)
110    energy.append(en/N)
111
112
113    to_sum = 0
114    for j in range(N):
115        to_sum += (- (alpha[i]**2)/2 + alpha[i]/np.linalg.norm(r[j]) -
116                    1/np.linalg.norm(r[j]) - energy[i])**2
117
118
119    std_dev.append(np.sqrt(to_sum)/np.sqrt(N))
120
121    '''
122    if i == 1:
123        axes2.hist([np.linalg.norm(i) for i in r], bins = 100, normed = True)
124        axes2.plot([n*.1 for n in range(0,3000)] , ,
125                  [2*alpha[i]*np.e**(-2*alpha[i]*n*.1) for n in range(0,3000)])
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128 #####
129 #####
130 #Plotting
131
132
133 std_dev = [sev/20 for sev in std_dev]
134
135 fig1, axes1 = plt.subplots()
136
137 #axes1.scatter(alpha, [3/2*num-2**(3/2)/(np.pi**.5)*num**.5 for num in alpha])
138 #axes1.scatter(8/(9*np.pi), 3/2*(8/(9*np.pi))-2**(3/2)/(np.pi**.5)*(8/(9*np.pi))**.5)
139 #axes1.plot(alpha, energy)
140 axes1.errorbar(alpha, energy, yerr=std_dev, fmt='o', linestyle='-')
141 axes1.plot(alpha, [num**2-27*num/8 for num in alpha])
142
143 axes1.set_ylabel('Energy')
144 axes1.set_xlabel('alpha')
145 axes1.set_title("Energy vs alpha", va='bottom')
146
147
148 plt.show()

```